Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.53e-09 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.55e-01

Confidence level: 5.54e-01

Nearest Neighbors from the Training Set

Image not found
Pentadecane
Measured: 3.58e-10
Predicted: 1.53e-09

Image not found
Hexadecane
Measured: 3.97e-09
Predicted: 4.12e-09

Image not found
Tetradecane
Measured: 1.97e-08
Predicted: 1.05e-08

Image not found
Tridecane
Measured: 2.55e-08
Predicted: 1.55e-08

Image not found
Octadecane
Measured: 2.36e-08
Predicted: 1.34e-08